



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:36 AM UTC

PDB ID : 7Z8G / pdb_00007z8g
EMDB ID : EMD-14550
Title : Cytoplasmic dynein-1 motor domain
Authors : Chaaban, S.; Carter, A.P.
Deposited on : 2022-03-17
Resolution : 3.52 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

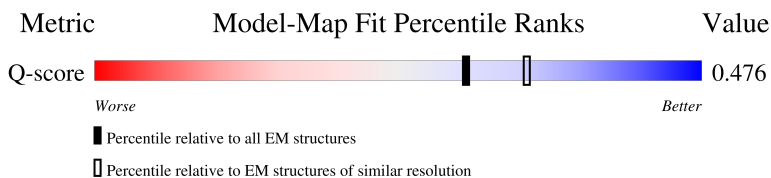
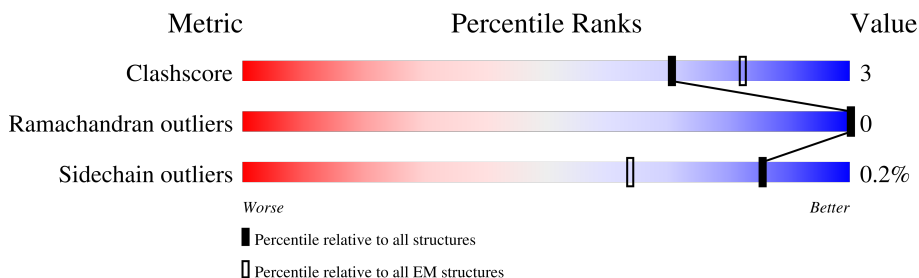
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13017 (3.02 - 4.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	18% 60% 6% 34%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

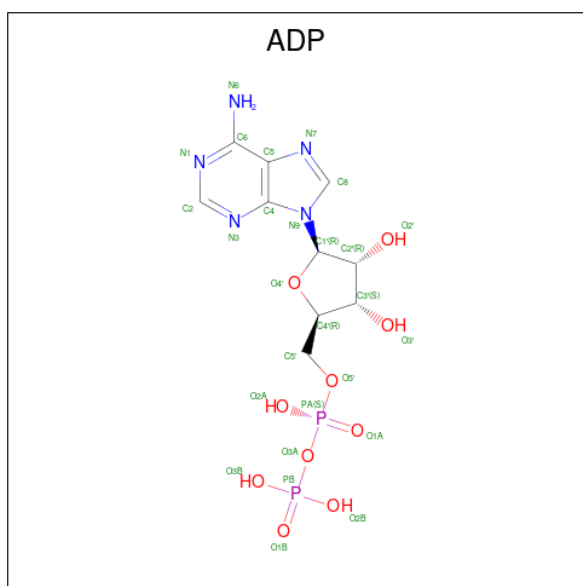
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3047	24535	15622	4234	4557	122	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1567	GLU	ARG	engineered mutation	UNP Q14204
A	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

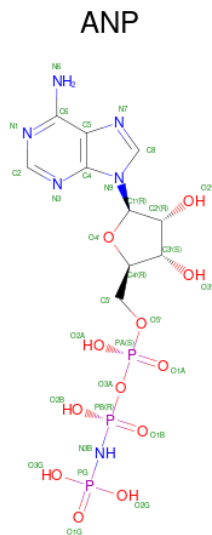


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0

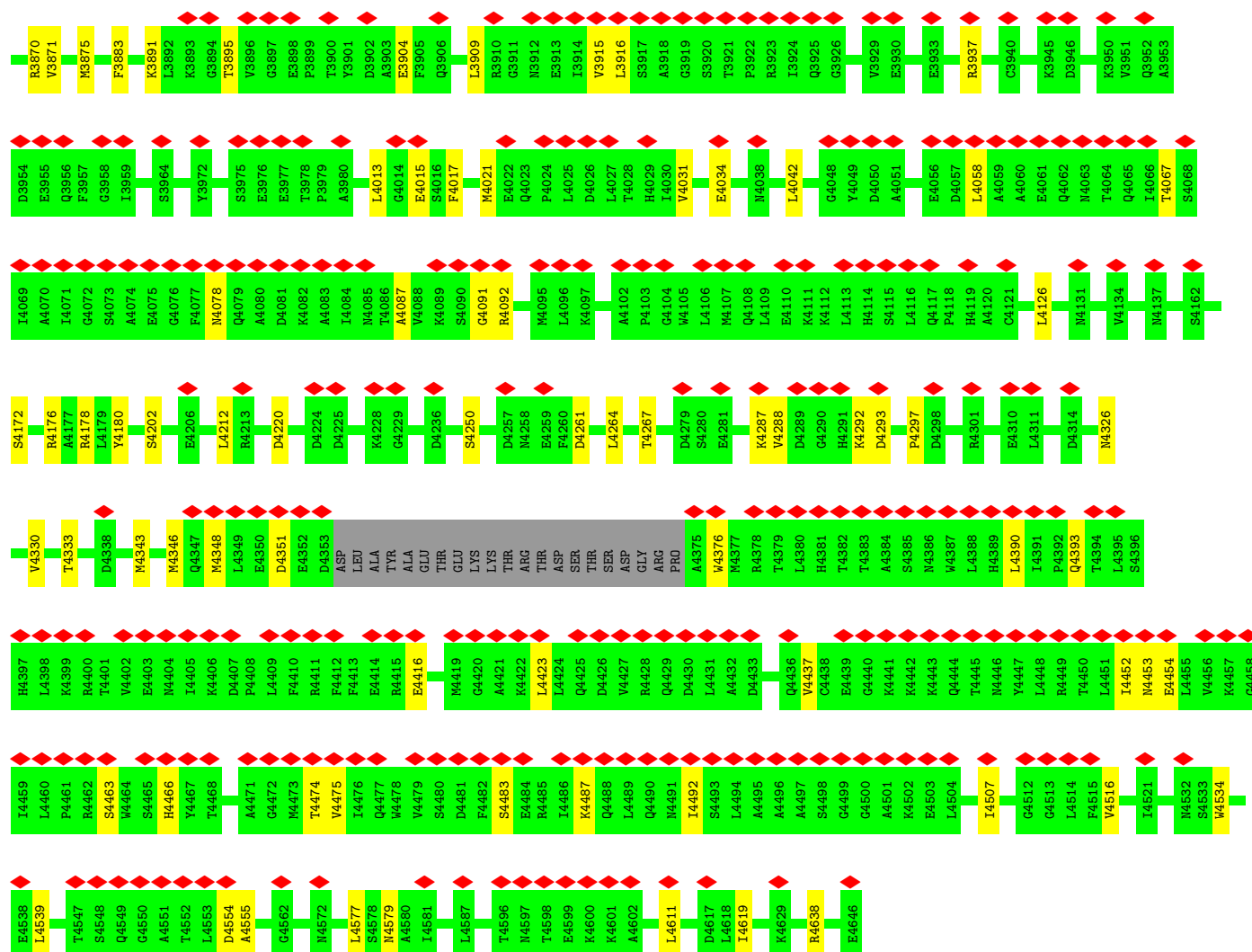
- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	

V2247	D2255	K2114	H1985	G1770	I1550	A1444	S1382	VAL	TRP	ARG	GLU	ALA	ASN	GLU	ASN	PHE
E2248	P2256	K2115	S1986	G1771	F1551	I1445	Y1383	ALA	GLU	PHE	PHE	LEU	LYS	LEU	LYS	ASN
G2249	K2257	E2116	N1987	G1772	T1552	V1446	E1384	GLU	THR	PHE	THR	VAL	GLN	ASP	GLN	PHE
D2255	A2258	E2117	P1988	G1773	G1553	K1447	F1385	LEU	VAL	PRO	ASN	ILE	GLY	VAL	LYS	GLY
P2256	K2257	K2118	N1989	D1774	S1554	D1448	Q1386	Q1327	THR	TRP	SER	ARG	PRO	ASP	VAL	VAL
K2257	A2258	K2119	Y1990	A1775	A1555	V1449	R1388	D1328	GLY	TYR	LEU	LYS	GLY	ASP	ASP	ASP
A2258		E2120	D1991		D1556	L1450	L1389	L1329	ASN	TYR	GLN	ARG	VAL	LEU	LEU	LEU
K2261		A2121	K1992	D1794	K1558	L1451	L1390	K1330	ARG	ASN	ASN	THR	ALA	GLY	ILE	ILE
D2262		D2122	T1993	M1798	H1559	E1456	K1391	W1333	PRO	ILE	PRO	VAL	LEU	VAL	PRO	GLU
H2263		E2123	E1799	E1799	E1564	E1460	G1392	S1334	GLU	GLU	GLU	ASP	GLU	ARG	GLU	GLU
G2266		E2124	L1803		I1571	E1461	Y1393	S1335	ALA	GLY	GLN	ASN	GLU	LEU	LEU	GLY
T2267		G2125	R1804		A1577	F1462	M1394	L1336	LEU	GLU	SER	THR	TYR	ALA	ILE	ILE
L2268		E2129	R1805		D1590	L1463	K1395	S1337	GLN	GLY	SER	THR	SER	VAL	GLY	ASP
D2269		W2130	R1806		D1590	K1464	I1397	K1338	ALA	GLY	ARG	VAL	ARG	LEU	LEU	LEU
D2270		E2133	H1810		R1599	Q1465	M1398	W1339	LEU	PHE	THR	ALA	MET	GLU	GLU	VAL
P2270		Q2134	D1847		E1602	I1472	I1401	E1341	ALA	ILE	SER	PRO	VAL	VAL	GLU	GLU
K2004		E2135	P1848		D1606	Y1473	L1403	E1342	THR	ARG	GLY	VAL	GLU	VAL	LEU	VAL
K2004		E2135	K1849		L1607	E1474	E1403	I1343	ILE	LYS	LYS	ILE	VAL	VAL	LEU	GLU
K2004		E2135	P1848		L1607	L1475	S1405	D1344	THR	ARG	THR	ASP	GLY	GLN	GLY	ALA
K2004		E2135	K1849		L1607	D1476	E1406	Q1345	ARG	ASP	PHE	THR	GLN	TRP	TRP	ALA
K2004		E2135	K1849		L1607	D1476	E1407	M1346	LEU	SER	ILE	LYS	VAL	VAL	ALA	ASP
K2004		E2135	K1849		L1607	D1476	A1407	K1347	LYS	ILE	THR	VAL	VAL	VAL	GLY	GLY
K2004		E2135	K1849		L1607	D1476	L1408	E1348	ASP	ILE	TYR	VAL	VAL	VAL	MET	GLU
K2004		E2135	K1849		L1607	D1476	K1409	E1348	ASP	GLN	VAL	GLN	VAL	VAL	LEU	THR
K2004		E2135	K1849		L1607	D1476	D1410	E1348	ASP	GLN	VAL	GLN	VAL	VAL	LEU	THR
K2004		E2135	K1849		L1607	D1476	R1411	P1350	GLU	GLU	SER	GLY	GLN	VAL	GLY	ALA
K2004		E2135	K1849		L1607	D1476	R1411	W1351	VAL	VAL	VAL	ASN	GLN	VAL	ASP	ILE
K2004		E2135	K1849		L1607	D1476	R1411	V1352	CYS	ALA	ARG	LEU	GLN	VAL	MET	LEU
K2004		E2135	K1849		L1607	D1476	R1411	S1353	ALA	ASN	ARG	LEU	CYS	ASN	ASP	ASN
K2004		E2135	K1849		L1607	D1476	R1411	V1354	LYS	LEU	ILE	LYS	THR	THR	THR	ASN
K2004		E2135	K1849		L1607	D1476	R1411	Q1355	LYS	GLN	TRP	TRP	VAL	VAL	ASP	VAL
K2004		E2135	K1849		L1607	D1476	R1411	P1356	GLU	LYS	SER	GLN	GLN	GLN	ALA	GLN
K2004		E2135	K1849		L1607	D1476	R1411	R1357	ALA	ILE	ARG	TRP	PRO	VAL	PRO	LYS
K2004		E2135	K1849		L1607	D1476	R1411	K1358	GLU	VAL	GLN	GLN	GLN	ALA	ALA	VAL
K2004		E2135	K1849		L1607	D1476	R1411	L1359	GLU	GLU	VAL	GLU	VAL	VAL	VAL	VAL
K2004		E2135	K1849		L1607	D1476	R1411	L1360	THR	ASP	GLY	GLY	GLY	GLY	ASP	ASP
K2004		E2135	K1849		L1607	D1476	R1411	Q1361	THR	ALA	THR	VAL	VAL	VAL	ASN	ASN
K2004		E2135	K1849		L1607	D1476	R1411	M1362	GLY	VAL	ARG	GLY	GLY	GLY	GLY	HIS
K2004		E2135	K1849		L1607	D1476	R1411	L1363	LEU	SER	ASN	LEU	LEU	LEU	GLY	GLY
K2004		E2135	K1849		L1607	D1476	R1411	D1364	LEU	ARG	GLY	GLY	GLY	GLY	GLY	GLY
K2004		E2135	K1849		L1607	D1476	R1411	A1365	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	L1366	SER	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	L1367	GLU	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	M1368	GLU	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	Q1369	VAL	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	L1370	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	K1371	SER	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	S1372	GLU	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	F1373	GLU	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	A1375	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	R1376	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	L1377	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	Q1440	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	K1441	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	M1442	GLY	THR	THR	THR	THR	THR	THR	THR
K2004		E2135	K1849		L1607	D1476	R1411	E1443	GLY	THR	THR	THR	THR	THR	THR	THR





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.076	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0325	Depositor
Map size (Å)	843.77106, 843.77106, 843.77106	wwPDB
Map dimensions	678, 678, 678	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2445, 1.2445, 1.2445	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, ADP, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/25054	0.35	0/33945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	24535	0	24579	169	0
2	A	27	0	12	0	0
3	A	31	0	12	5	0
4	A	1	0	0	0	0
5	A	62	0	26	4	0
All	All	24656	0	24629	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2729:ARG:NH1	3:A:4702:ATP:O2G	2.22	0.73
1:A:1336:LEU:HD11	1:A:1386:VAL:HG21	1.71	0.72
1:A:2801:ARG:NH2	1:A:3087:ASN:O	2.23	0.72
1:A:1483:LYS:NZ	1:A:1548:GLU:OE2	2.23	0.71
1:A:2453:ARG:NH2	1:A:2505:ASP:OD2	2.23	0.71
1:A:3194:LEU:HD22	1:A:3500:MET:HE1	1.72	0.70
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.26	0.68
1:A:4288:VAL:N	1:A:4292:LYS:O	2.26	0.68
1:A:2295:LEU:O	1:A:2338:ASN:ND2	2.28	0.67
1:A:2409:ALA:HB3	1:A:2413:LEU:HD12	1.75	0.67
1:A:2172:ARG:NH1	1:A:2205:GLU:OE2	2.27	0.66
1:A:1649:LYS:O	1:A:1652:LYS:NZ	2.27	0.66
1:A:3767:ILE:O	1:A:3771:GLU:N	2.29	0.65
1:A:4453:ASN:ND2	1:A:4454:GLU:OE2	2.29	0.65
1:A:3544:ARG:NH2	1:A:3546:ASP:OD1	2.30	0.64
1:A:2999:VAL:O	1:A:3078:ARG:NH1	2.30	0.64
1:A:2609:LEU:HD22	1:A:2660:VAL:HG11	1.80	0.64
1:A:4423:LEU:HD13	1:A:4466:HIS:CE1	2.33	0.63
1:A:2581:LEU:HD11	1:A:2605:LEU:HD23	1.80	0.62
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.32	0.62
1:A:3486:ARG:NH2	1:A:3487:GLU:OE2	2.32	0.62
1:A:3113:MET:O	1:A:3140:ARG:NH2	2.33	0.62
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.82	0.61
1:A:3116:GLU:OE2	1:A:3140:ARG:NH1	2.33	0.61
5:A:4705:ANP:O1G	5:A:4705:ANP:O2B	2.18	0.61
1:A:4483:SER:OG	1:A:4487:LYS:NZ	2.34	0.60
1:A:2207:VAL:HG22	1:A:2237:LEU:HD13	1.83	0.60
1:A:3909:LEU:HD21	1:A:4343:MET:HE2	1.84	0.59
1:A:3627:LEU:HD21	1:A:3662:ILE:HG21	1.85	0.59
1:A:4172:SER:O	1:A:4176:ARG:NH1	2.36	0.59
1:A:2579:ALA:O	1:A:2583:THR:HG23	2.01	0.59
1:A:3712:CYS:O	1:A:3716:VAL:HG23	2.02	0.59
1:A:2987:ASN:ND2	1:A:3057:GLN:OE1	2.35	0.58
1:A:3492:THR:O	1:A:3495:THR:OG1	2.21	0.58
1:A:2747:ILE:O	1:A:2750:THR:OG1	2.18	0.57
1:A:2934:LEU:HD12	1:A:3066:PHE:HB2	1.84	0.57
1:A:2695:THR:O	1:A:2698:GLN:NE2	2.37	0.57
1:A:2995:ASP:OD1	1:A:3067:THR:OG1	2.22	0.57
1:A:3875:MET:HE1	1:A:3883:PHE:HB2	1.86	0.57
1:A:1564:GLU:N	1:A:1564:GLU:OE1	2.37	0.56
1:A:1752:LEU:HD11	1:A:1868:TYR:CZ	2.39	0.56
1:A:2393:GLU:N	1:A:2393:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2762:LEU:HD23	1:A:2821:LEU:HD22	1.88	0.56
1:A:2624:SER:N	1:A:3006:GLU:OE2	2.38	0.56
1:A:2661:LEU:HD12	1:A:2708:PHE:CE2	2.41	0.56
1:A:2593:LEU:CD1	1:A:2605:LEU:HD21	2.37	0.55
1:A:2726:ARG:NH1	3:A:4702:ATP:O1G	2.39	0.55
1:A:2943:LYS:NZ	5:A:4705:ANP:O2G	2.37	0.55
1:A:4021:MET:HA	1:A:4021:MET:HE2	1.89	0.55
1:A:1443:GLU:N	1:A:1443:GLU:OE1	2.40	0.55
1:A:2766:ALA:O	1:A:2770:THR:HG23	2.07	0.55
1:A:3086:PHE:O	1:A:3091:LEU:HD11	2.07	0.54
1:A:3482:LEU:HD23	1:A:3770:LEU:HD11	1.88	0.54
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.89	0.54
1:A:2726:ARG:NH2	3:A:4702:ATP:O3G	2.40	0.54
1:A:4015:GLU:N	1:A:4015:GLU:OE1	2.40	0.54
1:A:3580:LEU:HD13	1:A:3600:ILE:HD11	1.89	0.54
1:A:4474:THR:OG1	1:A:4475:VAL:N	2.41	0.54
1:A:2223:VAL:HG13	1:A:2345:VAL:HG23	1.90	0.54
1:A:4042:LEU:CD2	1:A:4126:LEU:HD12	2.38	0.53
1:A:3891:LYS:O	1:A:3895:THR:N	2.42	0.53
1:A:4492:ILE:HD13	1:A:4507:ILE:HG21	1.90	0.53
1:A:2223:VAL:HG13	1:A:2345:VAL:CG2	2.40	0.52
1:A:2287:ILE:HD13	1:A:2339:VAL:HG22	1.91	0.52
1:A:3162:ALA:HB2	1:A:3168:THR:HG21	1.92	0.52
1:A:2559:THR:HG22	1:A:2754:ALA:O	2.09	0.52
1:A:3211:THR:HG21	1:A:3753:LEU:HD11	1.92	0.52
1:A:2836:ARG:NH1	1:A:3091:LEU:HD13	2.25	0.52
1:A:3194:LEU:HD22	1:A:3500:MET:CE	2.39	0.52
1:A:1571:ILE:HD11	1:A:1607:LEU:HB3	1.92	0.51
1:A:3839:VAL:HG21	1:A:3863:LEU:HA	1.91	0.51
1:A:2587:GLU:OE1	1:A:2587:GLU:N	2.43	0.51
1:A:3190:LYS:CB	1:A:3503:ILE:HD11	2.41	0.51
1:A:4087:ALA:O	1:A:4091:GLY:N	2.43	0.51
1:A:2934:LEU:HD12	1:A:3066:PHE:CB	2.40	0.51
1:A:1711:VAL:HG22	1:A:1853:VAL:HG21	1.93	0.51
1:A:2776:PHE:HZ	1:A:2846:THR:HG23	1.75	0.51
1:A:2287:ILE:HD12	1:A:2299:GLN:OE1	2.11	0.51
1:A:4067:THR:OG1	1:A:4092:ARG:NH2	2.44	0.51
1:A:1429:LEU:HD21	1:A:1434:ILE:HD11	1.92	0.51
1:A:2601:LYS:NZ	5:A:4704:ANP:O2G	2.43	0.51
1:A:2666:ILE:HG22	1:A:2723:LEU:HD21	1.93	0.50
1:A:2686:MET:HG2	1:A:2703:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2999:VAL:O	1:A:2999:VAL:HG12	2.11	0.50
1:A:3473:ASN:O	1:A:3476:THR:OG1	2.25	0.50
1:A:2519:ARG:NH2	1:A:2527:PRO:O	2.44	0.50
1:A:4013:LEU:HD23	1:A:4017:PHE:CZ	2.46	0.49
1:A:3818:LEU:HD12	1:A:4346:MET:CE	2.42	0.49
1:A:1936:PHE:CE1	1:A:1941:MET:HE3	2.47	0.49
1:A:2603:MET:HE2	5:A:4704:ANP:H2'	1.94	0.49
1:A:2958:VAL:HG13	1:A:2993:ILE:HD12	1.94	0.49
1:A:2065:LEU:HD11	1:A:2133:GLU:HB3	1.94	0.49
1:A:1803:LEU:CD1	1:A:1875:VAL:HG21	2.42	0.49
1:A:2053:MET:O	1:A:2056:SER:OG	2.22	0.49
1:A:4463:SER:O	1:A:4466:HIS:NE2	2.44	0.49
1:A:1550:ILE:HD13	1:A:1615:LEU:HD21	1.93	0.48
1:A:1978:ILE:HG21	1:A:2014:ILE:HD12	1.96	0.48
1:A:3916:LEU:HD21	1:A:3937:ARG:HG2	1.95	0.48
1:A:2369:LEU:HD11	3:A:4702:ATP:C4	2.48	0.48
1:A:3190:LYS:HB2	1:A:3503:ILE:HD11	1.94	0.48
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.96	0.48
1:A:1891:THR:HG22	1:A:4250:SER:HA	1.96	0.48
1:A:1396:ILE:HD12	1:A:1439:LEU:HD12	1.94	0.48
1:A:2665:GLU:CB	1:A:2668:LEU:HD12	2.43	0.48
1:A:3692:LEU:O	1:A:3696:VAL:HG12	2.13	0.48
1:A:1336:LEU:CD1	1:A:1386:VAL:HG21	2.43	0.47
1:A:4437:VAL:HG11	1:A:4452:ILE:HD11	1.95	0.47
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.97	0.47
1:A:4348:MET:HE3	1:A:4351:ASP:O	2.15	0.47
1:A:2753:ARG:O	1:A:2763:ARG:NH2	2.48	0.47
1:A:3734:LEU:O	1:A:3739:GLN:NE2	2.48	0.47
1:A:3823:PHE:O	1:A:3826:GLN:NE2	2.48	0.47
1:A:1936:PHE:CZ	1:A:1941:MET:HE3	2.50	0.47
1:A:3875:MET:HE1	1:A:3883:PHE:CB	2.43	0.47
1:A:2234:TRP:CZ2	1:A:2302:VAL:HG21	2.50	0.47
1:A:2694:ARG:O	1:A:2698:GLN:N	2.48	0.47
1:A:3627:LEU:HD23	1:A:3669:ILE:CD1	2.44	0.47
1:A:3708:LEU:HD11	1:A:3829:LEU:HD11	1.95	0.47
1:A:2909:LEU:HD21	1:A:2945:THR:HG22	1.97	0.47
1:A:4348:MET:HE2	1:A:4376:TRP:HB3	1.97	0.47
1:A:1434:ILE:CG2	1:A:1439:LEU:HD11	2.45	0.47
1:A:2191:LEU:HD22	3:A:4702:ATP:C5	2.50	0.46
1:A:2448:ASP:O	1:A:2453:ARG:NH1	2.49	0.46
1:A:4180:TYR:OH	1:A:4220:ASP:OD2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4577:LEU:HD22	1:A:4638:ARG:HD2	1.97	0.46
1:A:4423:LEU:HD12	1:A:4423:LEU:O	2.16	0.46
1:A:2665:GLU:HB3	1:A:2668:LEU:HD12	1.98	0.46
1:A:1451:LEU:HD22	1:A:3673:PRO:HB3	1.97	0.46
1:A:1985:HIS:NE2	1:A:1997:ILE:HD13	2.31	0.46
1:A:3904:GLU:N	1:A:3904:GLU:OE1	2.49	0.46
1:A:2847:ASP:OD1	1:A:2869:ARG:NH1	2.49	0.45
1:A:3871:VAL:HG12	1:A:3875:MET:HE2	1.97	0.45
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.98	0.45
1:A:2958:VAL:CG1	1:A:2993:ILE:HD12	2.47	0.45
1:A:2464:GLN:HG2	1:A:2583:THR:HG22	1.99	0.45
1:A:2836:ARG:HH12	1:A:3091:LEU:HD13	1.81	0.44
1:A:2999:VAL:HG13	1:A:3005:LEU:HD21	1.99	0.44
1:A:4416:GLU:OE2	1:A:4516:VAL:HG12	2.18	0.44
1:A:1509:LEU:HD22	1:A:3608:LYS:HD2	2.00	0.44
1:A:4554:ASP:OD1	1:A:4555:ALA:N	2.47	0.44
1:A:1637:LEU:HD11	1:A:1641:ILE:HD11	2.00	0.44
1:A:1810:HIS:NE2	1:A:1876:GLN:O	2.51	0.44
1:A:2016:ILE:HD12	1:A:2036:PHE:CZ	2.53	0.44
1:A:2644:THR:OG1	1:A:2647:GLY:O	2.31	0.44
1:A:4330:VAL:O	1:A:4333:THR:HG22	2.18	0.44
1:A:4031:VAL:HG11	1:A:4058:LEU:HD21	1.99	0.43
1:A:3194:LEU:HD23	1:A:3194:LEU:O	2.19	0.43
1:A:4202:SER:OG	1:A:4261:ASP:OD2	2.28	0.43
1:A:4264:LEU:O	1:A:4267:THR:OG1	2.29	0.43
1:A:3500:MET:O	1:A:3503:ILE:HG22	2.19	0.43
1:A:2946:LEU:HD12	1:A:3094:PHE:HZ	1.83	0.43
1:A:4534:TRP:HE3	1:A:4539:LEU:HD21	1.84	0.42
1:A:2623:SER:O	1:A:2626:THR:HG22	2.18	0.42
1:A:3591:ASP:OD2	1:A:3597:THR:HG23	2.19	0.42
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.52	0.42
1:A:2957:SER:OG	1:A:2988:GLU:OE1	2.37	0.42
1:A:4423:LEU:HD13	1:A:4466:HIS:HE1	1.84	0.42
1:A:4287:LYS:N	1:A:4293:ASP:OD1	2.48	0.42
1:A:1518:GLU:OE1	1:A:1518:GLU:N	2.50	0.42
1:A:2214:THR:HG22	1:A:2220:LEU:HD21	2.02	0.42
1:A:1891:THR:HG21	1:A:2039:LEU:HD12	2.01	0.41
1:A:3870:ARG:NE	1:A:4034:GLU:OE1	2.53	0.41
1:A:4393:GLN:OE1	1:A:4393:GLN:N	2.53	0.41
1:A:3138:SER:OG	1:A:3139:HIS:N	2.54	0.41
1:A:1551:PHE:O	1:A:1558:LYS:NZ	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:MET:O	1:A:1805:ARG:NH2	2.54	0.40
1:A:3724:VAL:HG13	1:A:3794:VAL:HG12	2.03	0.40
1:A:1462:PHE:CZ	1:A:1466:ILE:HD11	2.56	0.40
1:A:3915:VAL:HG21	1:A:4390:LEU:HD21	2.04	0.40
1:A:2287:ILE:HD13	1:A:2339:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3039/4646 (65%)	2969 (98%)	70 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2710/4125 (66%)	2705 (100%)	5 (0%)	87	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1871	GLU

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Mol	Chain	Res	Type
1	A	3154	LEU
1	A	3588	LEU
1	A	4078	ASN
1	A	4212	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1670	ASN
1	A	1748	GLN
1	A	2130	ASN
1	A	2464	GLN
1	A	2531	ASN
1	A	2637	HIS
1	A	2886	GLN
1	A	2928	GLN
1	A	3185	ASN
1	A	3527	ASN
1	A	3988	HIS
1	A	4119	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ANP	A	4705	-	33,33,33	0.92	4 (12%)	45,52,52	0.63	0
5	ANP	A	4704	-	33,33,33	0.91	4 (12%)	45,52,52	0.64	0
2	ADP	A	4701	-	28,29,29	1.37	4 (14%)	43,45,45	1.95	10 (23%)
3	ATP	A	4702	4	32,33,33	0.65	1 (3%)	48,52,52	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	A	4705	-	-	5/18/38/38	0/3/3/3
5	ANP	A	4704	-	-	7/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	5/16/32/32	0/3/3/3
3	ATP	A	4702	4	-	2/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4701	ADP	C5-C4	4.42	1.47	1.39
5	A	4704	ANP	PB-O3A	-2.60	1.55	1.59
3	A	4702	ATP	PB-O3B	-2.56	1.56	1.59
5	A	4705	ANP	PG-O1G	2.49	1.50	1.46
2	A	4701	ADP	C5-N7	-2.48	1.34	1.39
2	A	4701	ADP	C5-C6	2.47	1.47	1.41
5	A	4704	ANP	PG-O1G	2.47	1.49	1.46
5	A	4705	ANP	PB-O3A	-2.44	1.56	1.59
5	A	4704	ANP	PG-N3B	2.32	1.69	1.63
5	A	4705	ANP	PG-N3B	2.28	1.69	1.63
5	A	4705	ANP	PB-O1B	2.27	1.49	1.46
2	A	4701	ADP	C8-N7	2.18	1.35	1.31
5	A	4704	ANP	PB-O1B	2.07	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-6.02	118.43	126.72
2	A	4701	ADP	N3-C4-N9	5.01	135.68	127.17
2	A	4701	ADP	C2-N3-C4	3.87	121.29	111.83
2	A	4701	ADP	N3-C2-N1	-3.68	123.00	128.58
2	A	4701	ADP	C4-C5-N7	-3.23	106.89	110.58
2	A	4701	ADP	C4-N9-C8	3.00	108.88	105.74
2	A	4701	ADP	C5-N7-C8	2.65	107.62	103.45
2	A	4701	ADP	C3'-C2'-C1'	2.37	105.95	101.46
2	A	4701	ADP	N9-C8-N7	-2.26	110.72	113.94
2	A	4701	ADP	C2'-C3'-C4'	2.04	106.55	102.61

There are no chirality outliers.

All (19) torsion outliers are listed below:

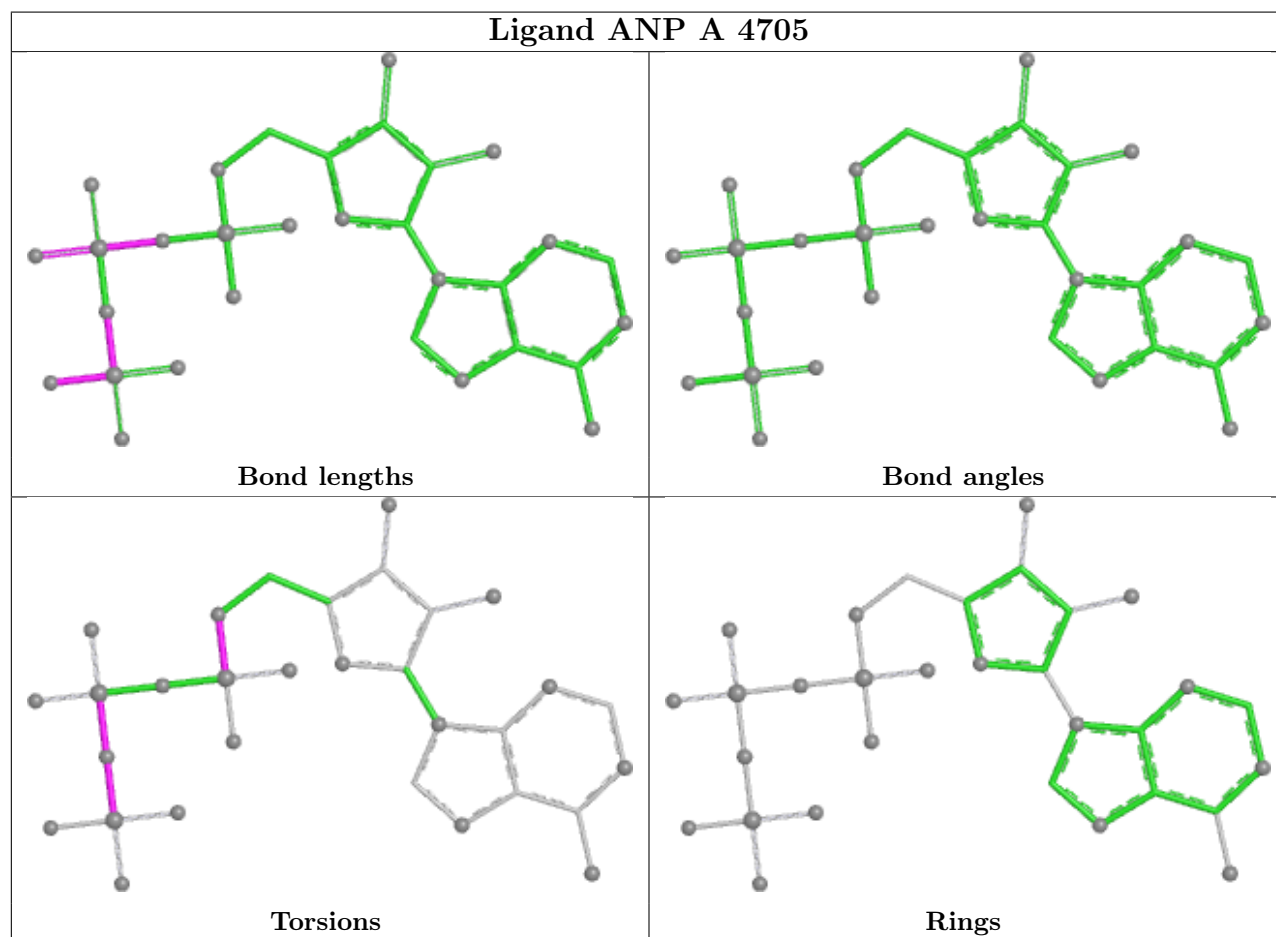
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	PA-O3A-PB-O2B
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
3	A	4702	ATP	PB-O3B-PG-O2G
5	A	4704	ANP	PG-N3B-PB-O1B
5	A	4704	ANP	PG-N3B-PB-O3A
5	A	4705	ANP	PB-N3B-PG-O1G
5	A	4705	ANP	PG-N3B-PB-O1B
5	A	4705	ANP	C5'-O5'-PA-O1A
5	A	4705	ANP	C5'-O5'-PA-O3A
5	A	4704	ANP	O4'-C4'-C5'-O5'
3	A	4702	ATP	PB-O3B-PG-O3G
5	A	4704	ANP	C3'-C4'-C5'-O5'
2	A	4701	ADP	C5'-O5'-PA-O1A
5	A	4704	ANP	C5'-O5'-PA-O1A
5	A	4704	ANP	C5'-O5'-PA-O2A
5	A	4704	ANP	C5'-O5'-PA-O3A
5	A	4705	ANP	C5'-O5'-PA-O2A
2	A	4701	ADP	PA-O3A-PB-O1B

There are no ring outliers.

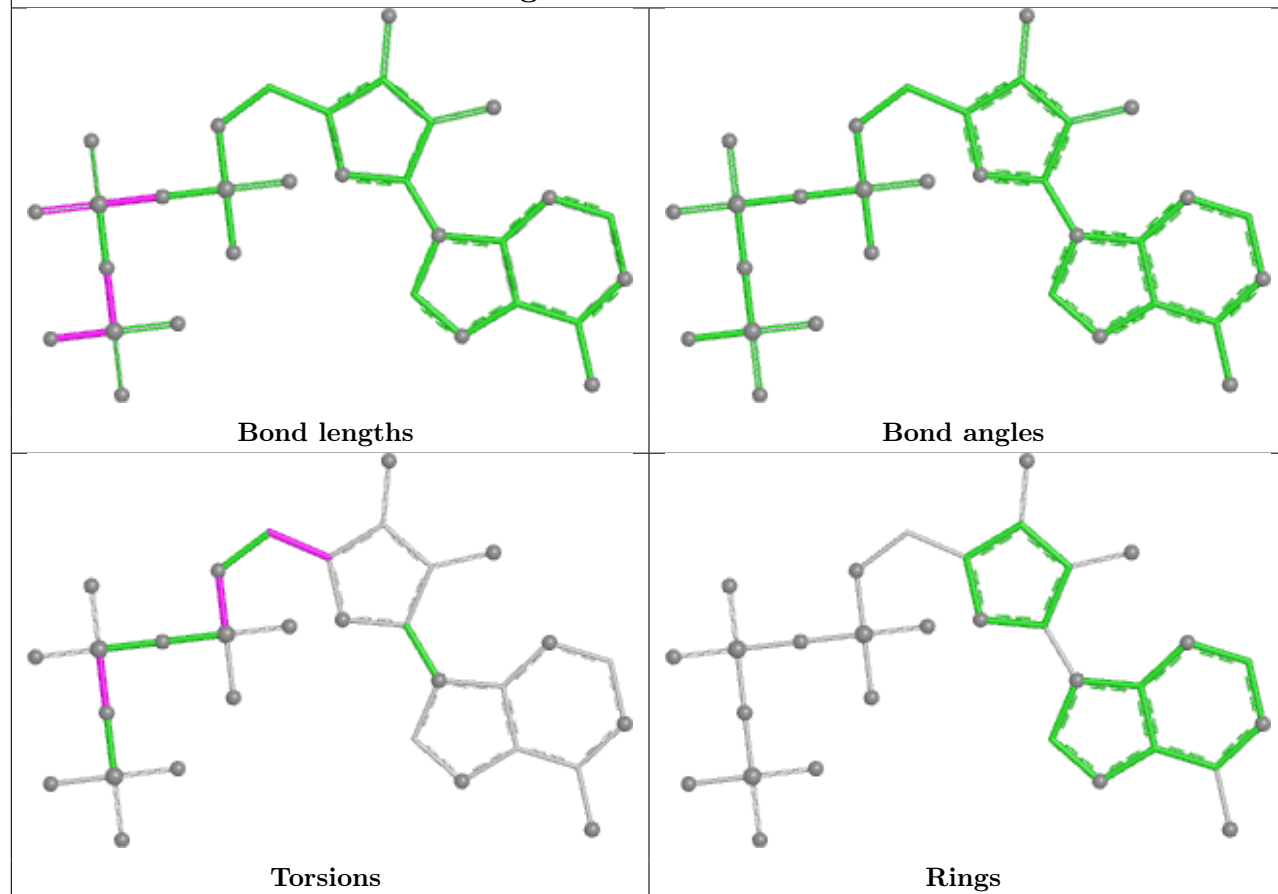
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	4705	ANP	2	0
5	A	4704	ANP	2	0
3	A	4702	ATP	5	0

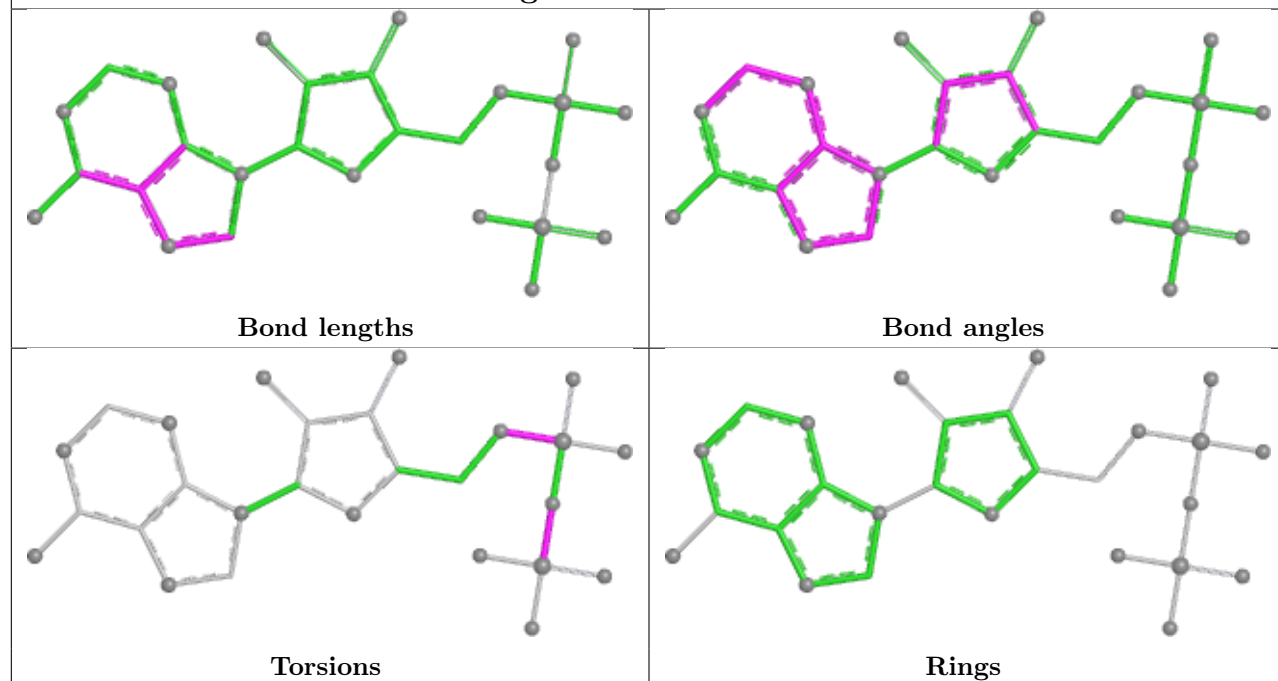
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

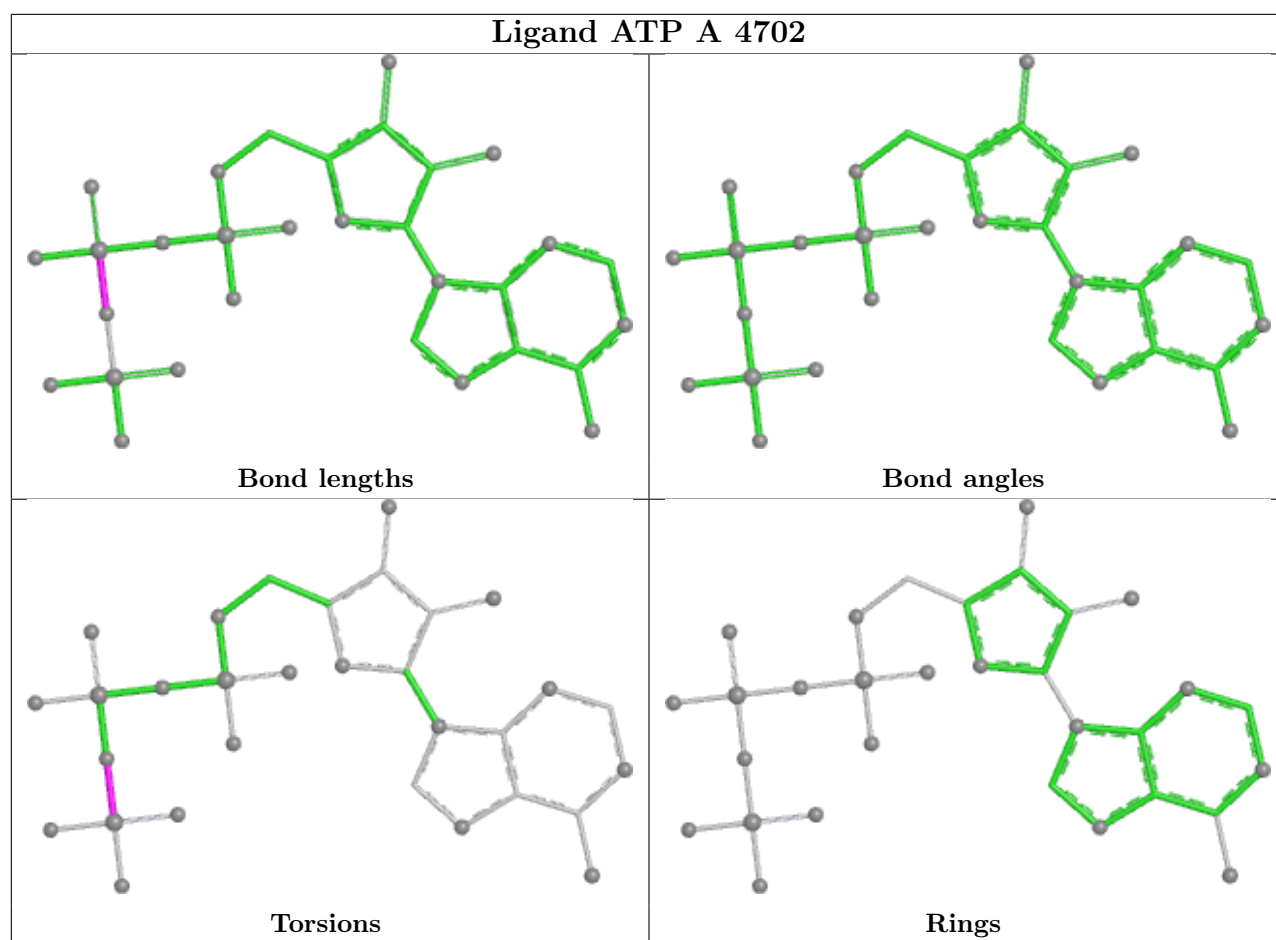


Ligand ANP A 4704



Ligand ADP A 4701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

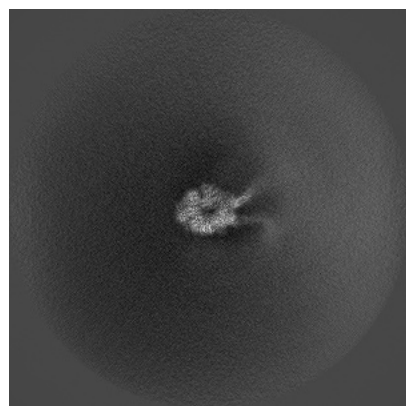
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14550. These allow visual inspection of the internal detail of the map and identification of artifacts.

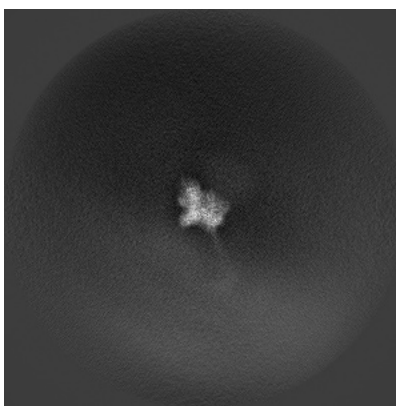
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

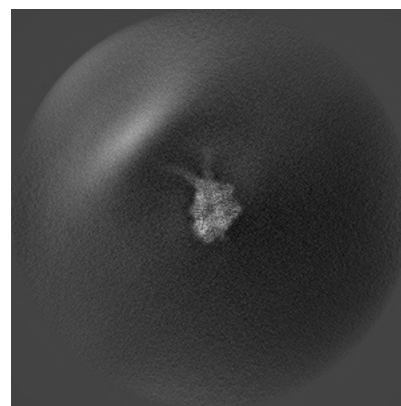
6.1.1 Primary map



X

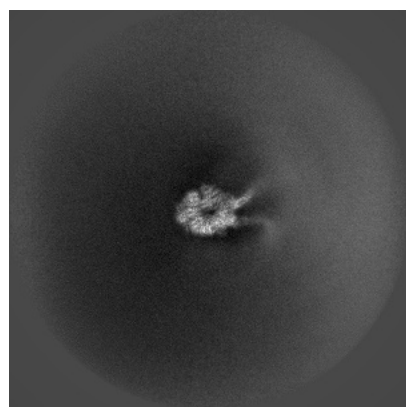


Y

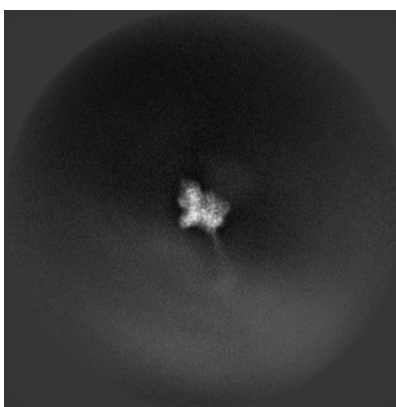


Z

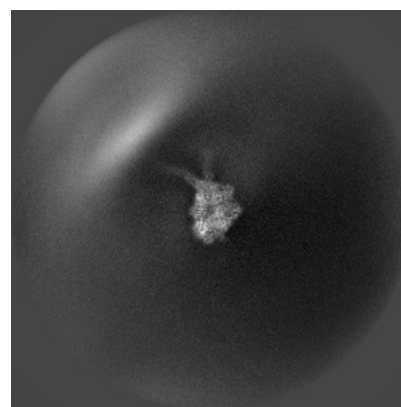
6.1.2 Raw map



X



Y



Z

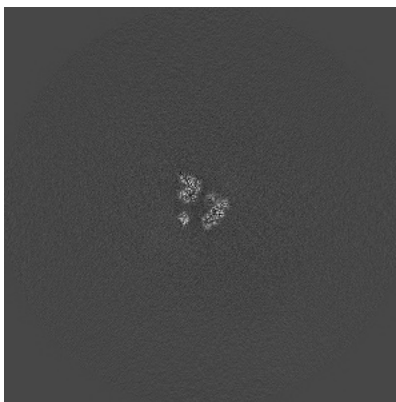
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

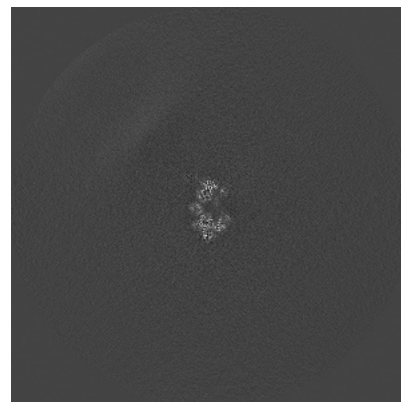
6.2.1 Primary map



X Index: 339



Y Index: 339

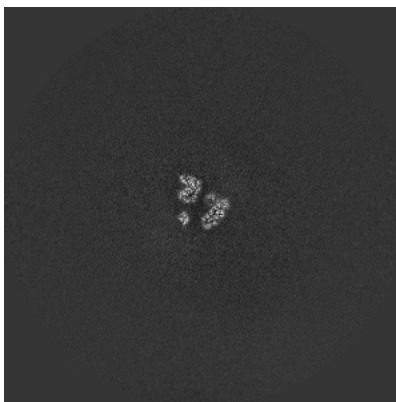


Z Index: 339

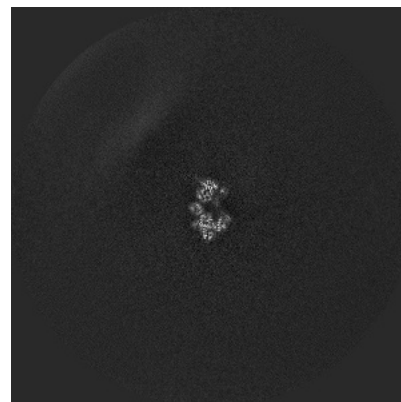
6.2.2 Raw map



X Index: 339



Y Index: 339

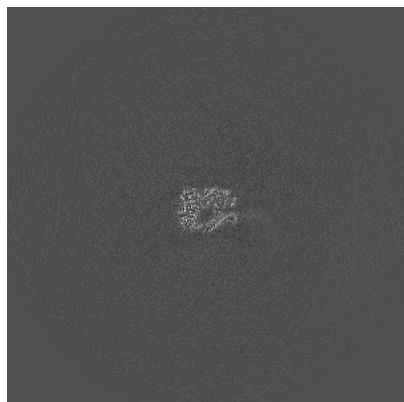


Z Index: 339

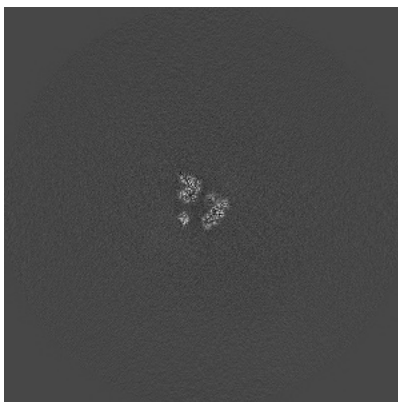
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

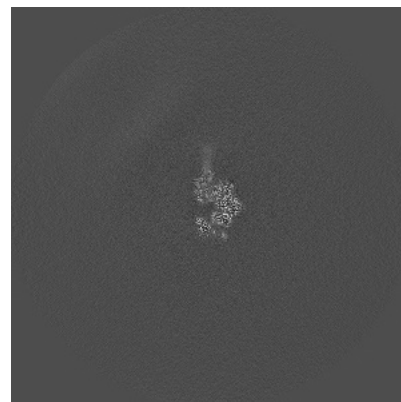
6.3.1 Primary map



X Index: 322

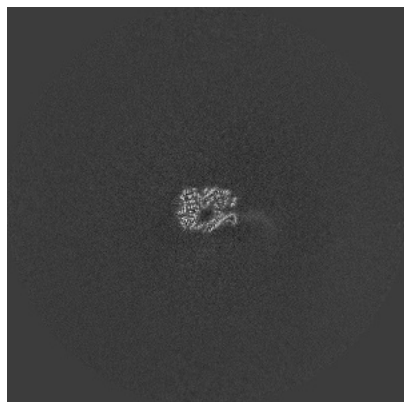


Y Index: 339

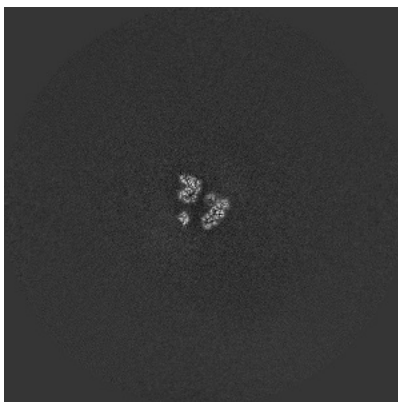


Z Index: 317

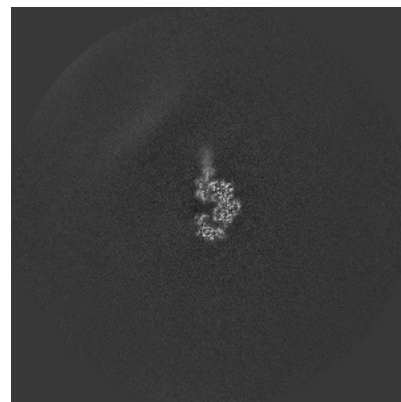
6.3.2 Raw map



X Index: 322



Y Index: 339

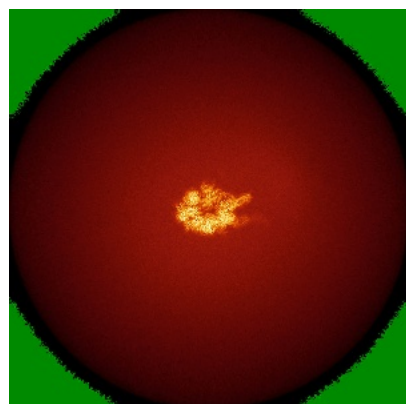


Z Index: 323

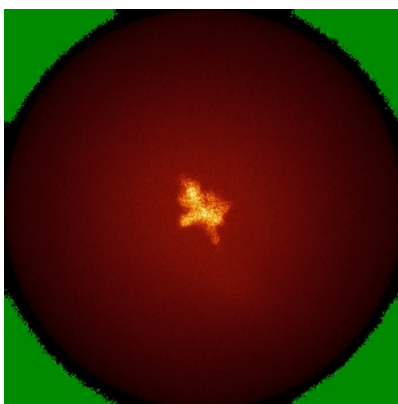
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

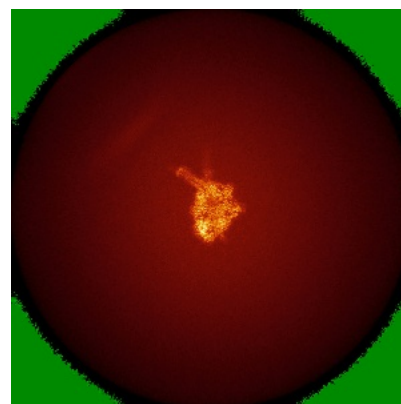
6.4.1 Primary map



X

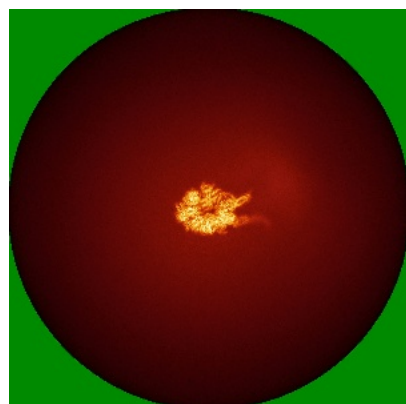


Y

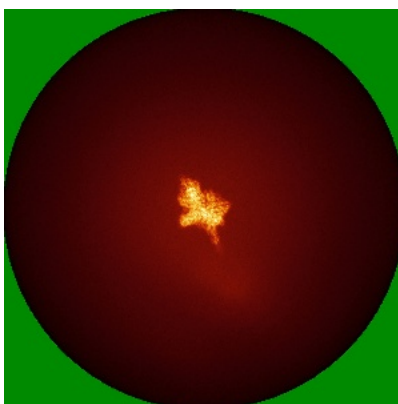


Z

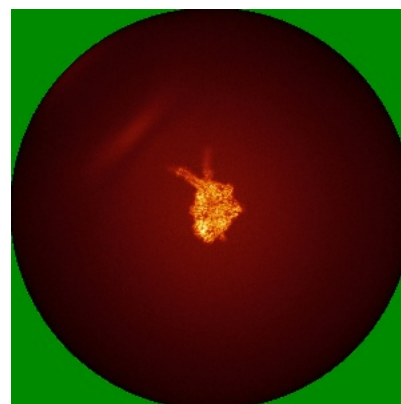
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

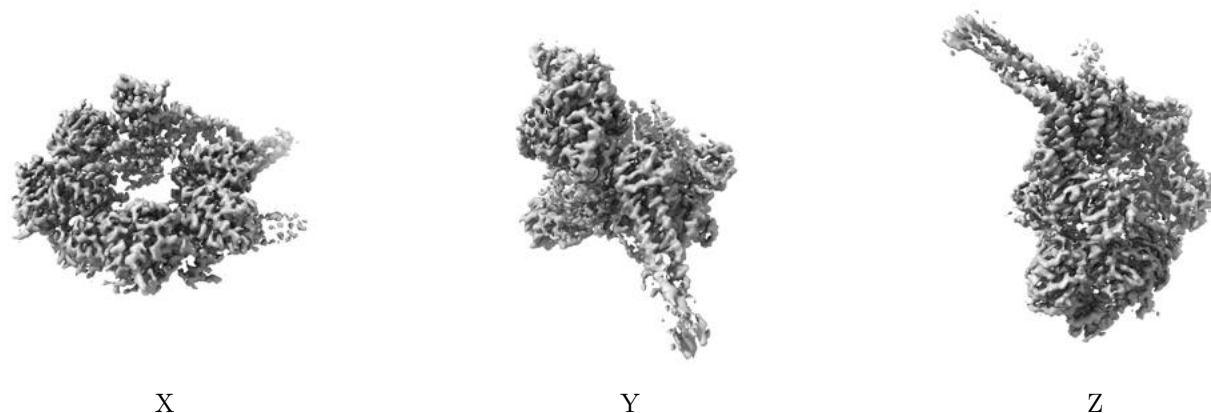
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0325. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

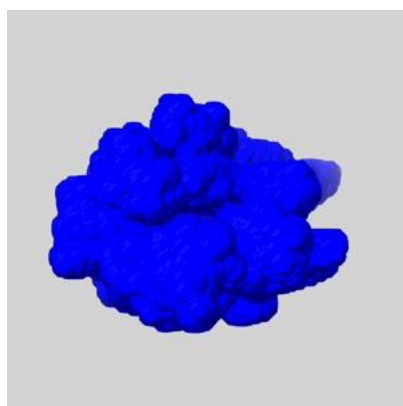
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

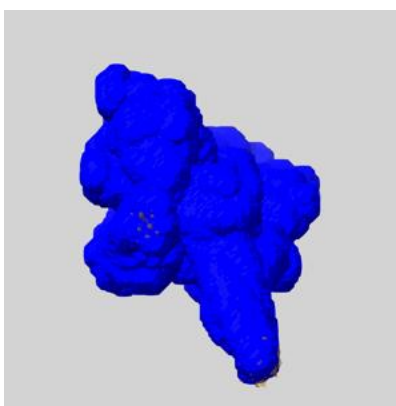
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

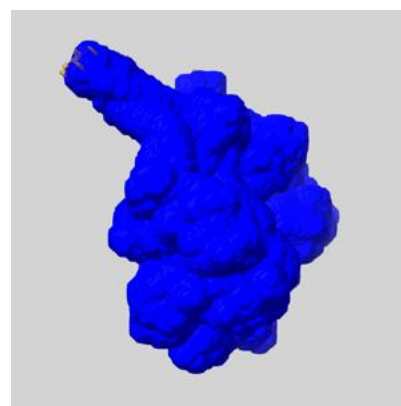
6.6.1 emd_14550_msk_1.map [i](#)



X



Y

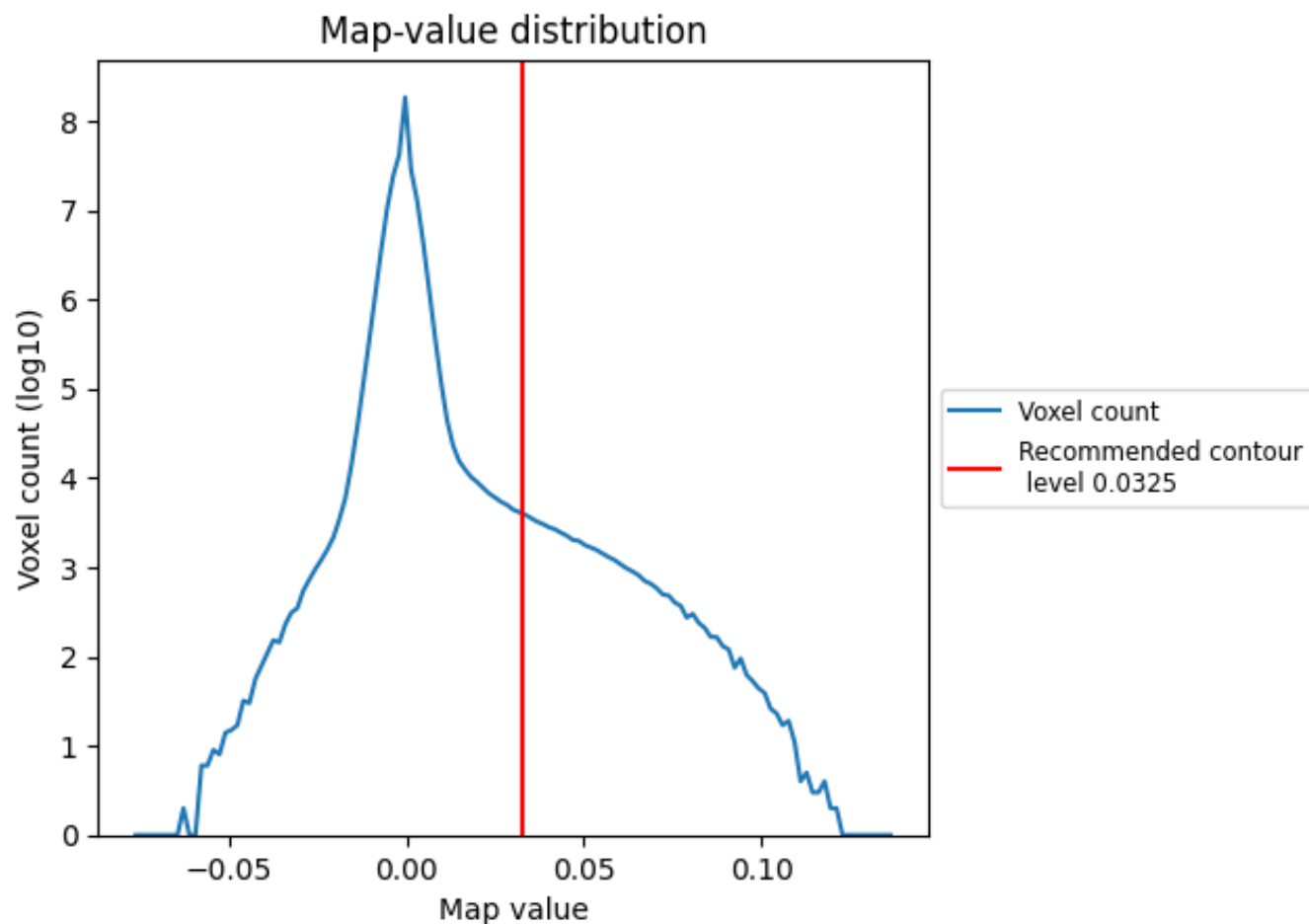


Z

7 Map analysis [i](#)

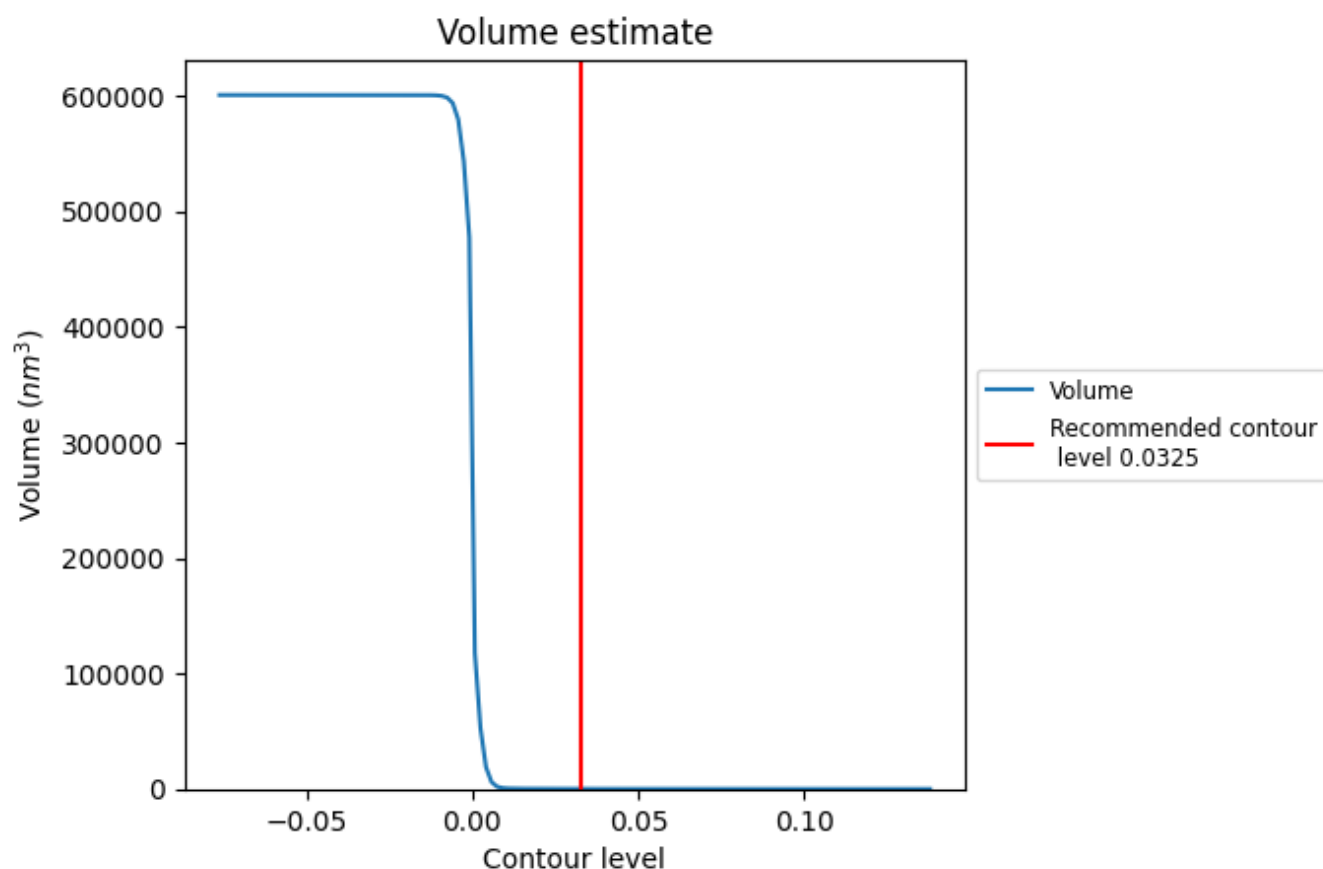
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

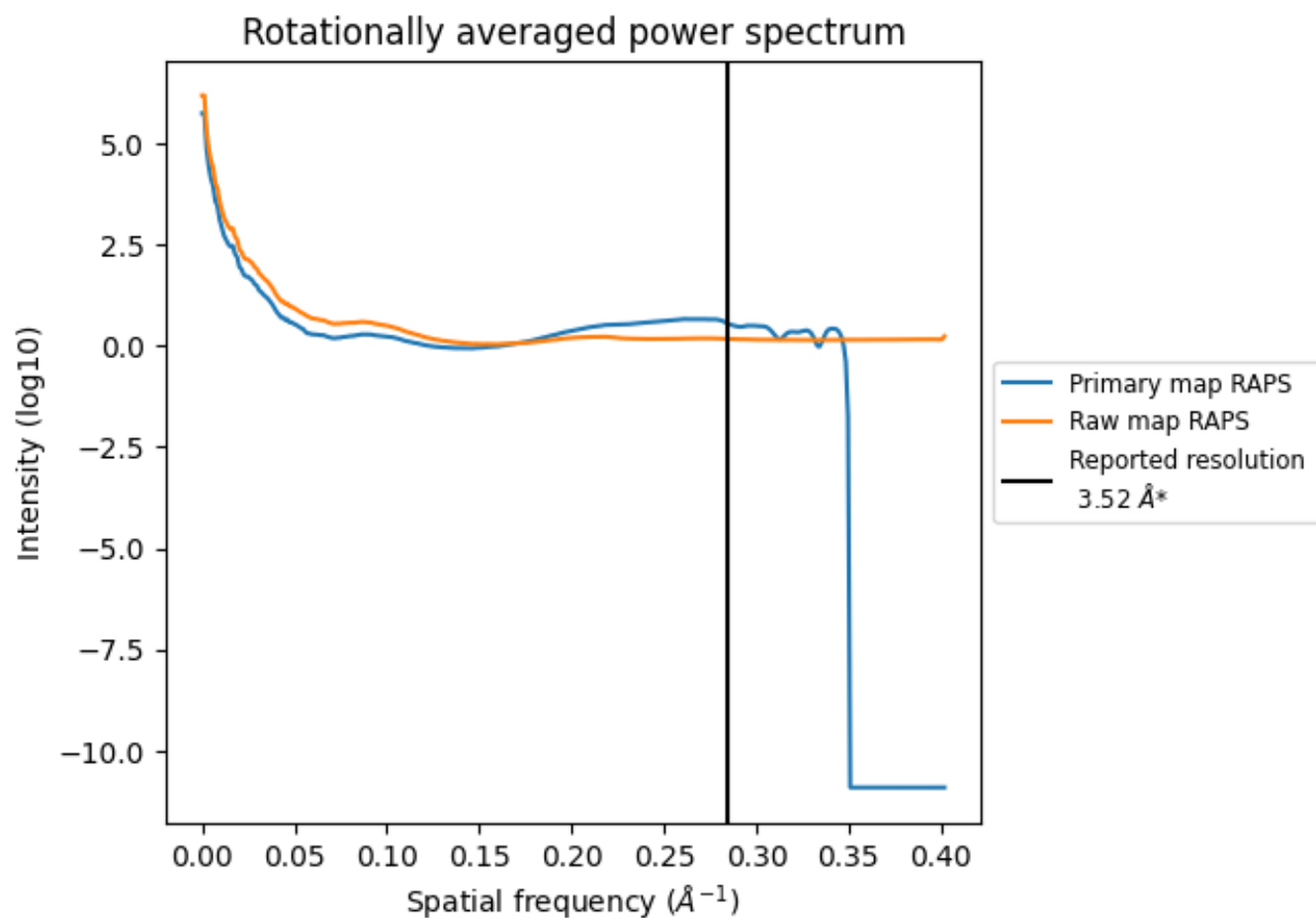
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

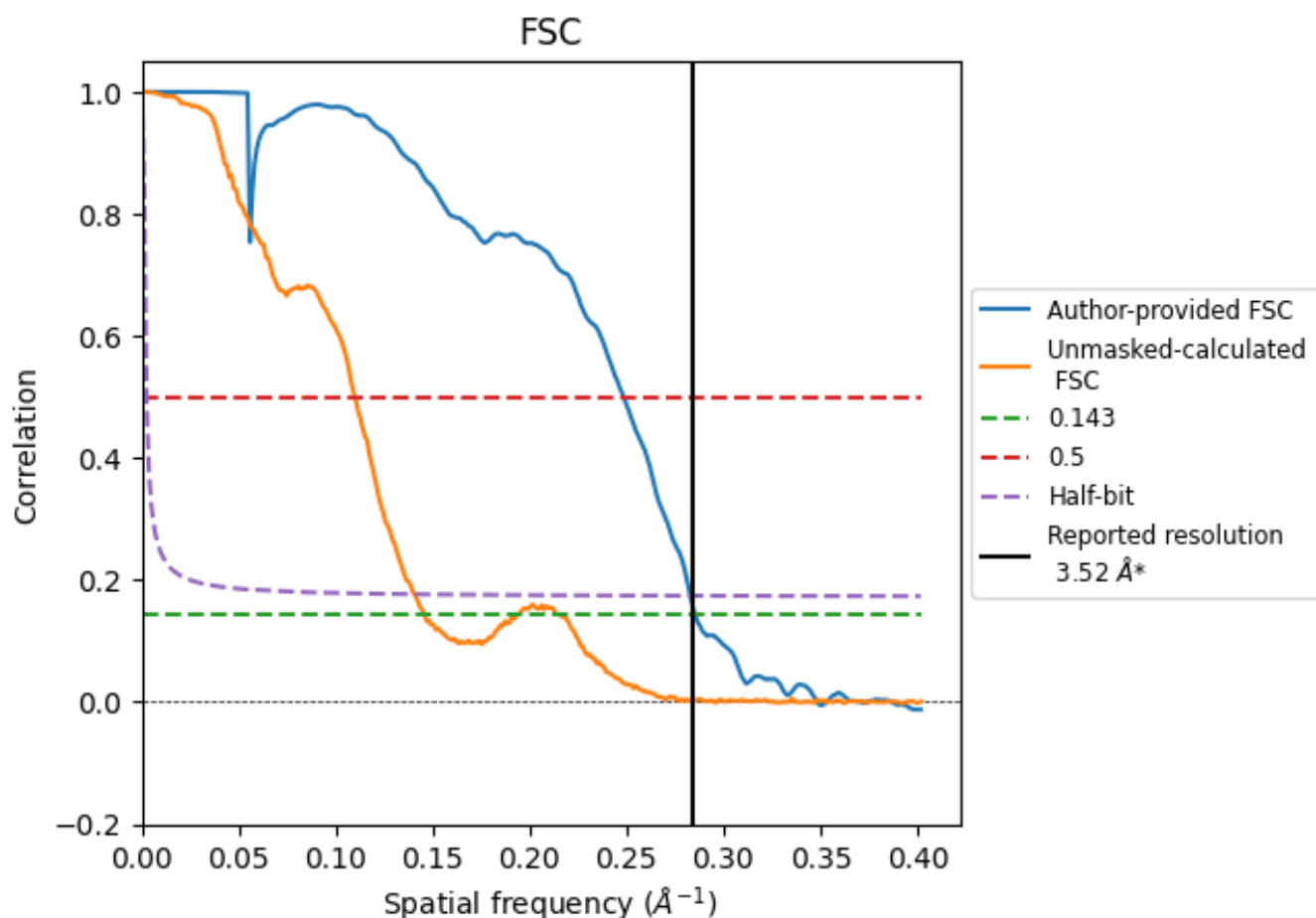


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.284 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	3.50	4.02	3.53
Unmasked-calculated*	6.86	9.11	7.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 3.52 by more than 10 %

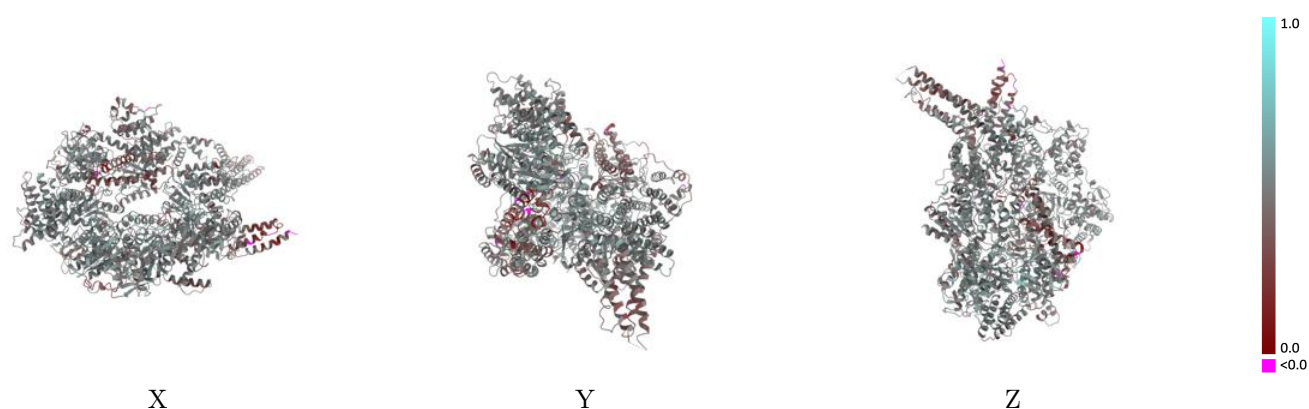
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14550 and PDB model 7Z8G. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

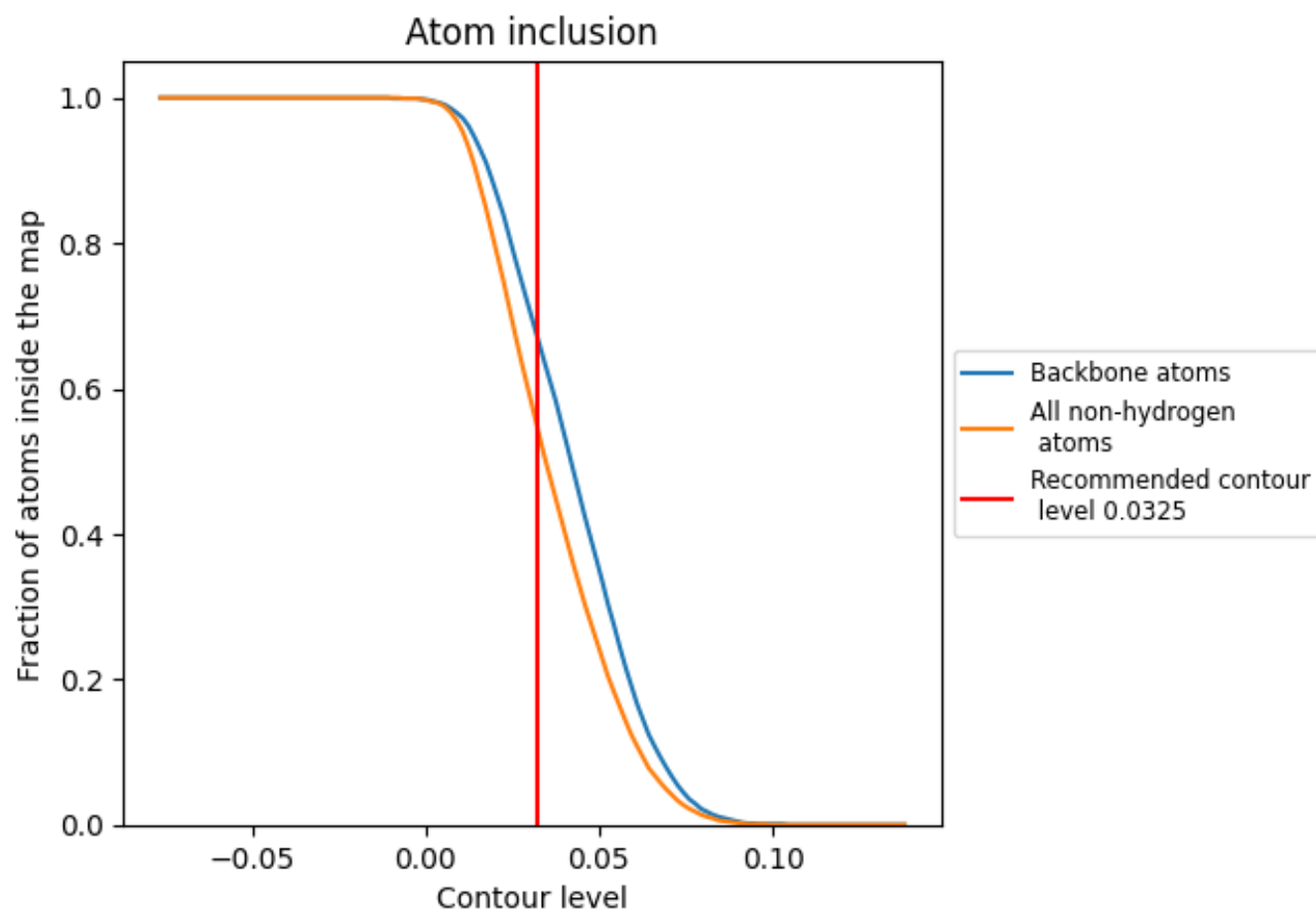


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0325) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.4760
A	0.5410	0.4760

